

Optical Excitation and Absorption Spectra of C_{2v} and D_{2d} Isomers of CO_4

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Recently the CO_4 isomer with C_{2v} symmetry has been detected in an experiment [C. S. Jamieson et al., Chem. Phys. Lett. **440**, 105 (2007)]. To further characterize this isomer, we report its optical excitation and absorption spectra calculated by the time-dependent density functional theory. Its rich spectral features are compared with those of another stable isomer having D_{2d} symmetry. Their spectral difference can be an evidence to distinguish the isomers in experiments.

Key words: CO_4 ; Vibrational Frequencies; Optical Excitation; Absorption Spectra.